②

AD-A206 683   DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1b. RESTRICTIVE MARKINGS

2a. SECURITY CLASSIFICATION AUTHORITY	3. DISTRIBUTION/AVAILABILITY OF REPORT
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE	Approved for public release; distribution is unlimited.

DTIC
ELECTE

4. PERFORMING ORGANIZATION REPORT NUMBER(S)

5. MONITORING ORGANIZATION REPORT NUMBER(S)

AFOSR·TR· 89-0418

6a. NAME OF PERFORMING ORGANIZATION	6b. OFFICE SYMBOL (if applicable)	7a. NAME OF MONITORING ORGANIZATION
Princeton University		AFOSR/NA
6c. ADDRESS (City, State, and ZIP Code)		7b. ADDRESS (City, State, and ZIP Code)
Princeton New Jersey 08544		Building 410, Bolling AFB DC 20332-6448

8a. NAME OF FUNDING/SPONSORING ORGANIZATION	8b. OFFICE SYMBOL (if applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER
AFOSR/NA	NA	AFOSR-85-0346

8c. ADDRESS (City, State, and ZIP Code)	10. SOURCE OF FUNDING NUMBERS			
Building 410, Bolling AFB DC 20332-6448	PROGRAM ELEMENT NO.	PROJECT NO.	TASK NO	WORK UNIT ACCESSION NO.
	61102F	2308	A2	

11. TITLE (Include Security Classification)

(U) Lumped Model Generation and Evaluation: Sensitivity and Lie Algebraic Techniques With Applications to Combustion

12. PERSONAL AUTHOR(S)

H. Rabitz, F. L. Dryer and R. Yetter

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Year, Month, Day)	15. PAGE COUNT
Final Technical	FROM 9/10/85 TO 11/30/89	89,03,03	9

16. SUPPLEMENTARY NOTATION

17.	COSATI CODES		18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB-GROUP	combustion modelling, sensitivity analysis, system lumping and reduction, Lie groups

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

This program dealt with the development and application of new approaches for producing and evaluating semi-empirical (lumped parameter) models of physical processes. Procedures using local sensitivity gradient methods were used to study the existing lumped kinetic models for the moist carbon monoxide oxidation to show that transport processes can cause oversimplified lumped models derived from homogeneous kinetics to fail when applied to flame propagation systems. New models are under development which will include the appropriate level of detail. A Lie group formalism was developed to address global parameter space mapping issues for first order differential equations. The rigorous criteria for the existence of exact lumping by linear projective transformations was also established.

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT	21. ABSTRACT SECURITY CLASSIFICATION
☒ UNCLASSIFIED/UNLIMITED ☒ SAME AS RPT. ☐ DTIC USERS	Unclassified
22a. NAME OF RESPONSIBLE INDIVIDUAL	22b. TELEPHONE (Include Area Code)	22c. OFFICE SYMBOL
Julian M Tishkoff	(202)767-0465	AFOSR/NA

DD Form 1473, JUN 86   Previous editions are obsolete.   SECURITY CLASSIFICATION OF THIS PAGE

Unclassified

AFOSR·TR· 89-0418

Abstract

Research under this program is aimed at setting out criteria for the ability to lump or reduce complex combustion kinetics systems. Research during this first phase of the project primarily focused on well stirred chemically reacting systems described by ordinary differential equations. The complexity of this problem necessitates a multi-faceted approach and three principal avenues of pursuit were considered. First, the tools of sensitivity analysis were employed to indicate particular portions of a chemical mechanism of importance as well as those which may be eliminated. In carrying forth this approach, an interesting and surprising level of scaling and self similarity was observed amongst the sensitivity coefficients strongly implying an ability to lump and reduce the models. Secondly, the rigorous criteria for lumping under a class of linear projective transformations were established. These criteria have utilities for a wide variety of nonlinear kinetic systems as well as other applications. Finally, a fully nonlinear approach to lumping and general system reduction was developed based on Lie group techniques. Each of these three approaches has its own realms of application and the research under this effort has clearly set the foundation for further development aimed ultimately at practical applications.

Accesion For		
NTIS CRA&I	☑	
DTIC TAB	☐	
Unannounced	☐	
Justification		
By		
Distribution /		
Availability Codes		
Dist	Avail and / or Special	
A-1		

Summary of Research Activities

Given below is a synopsis of the research carried out under this program. Each section summarizes a component of the research. The superscripts appearing in the section titles refer to specific papers which have appeared on these subjects. These references are summarized on page 8 of this report.

1. Scaling Relations and Self-Similarity Conditions in Strongly Coupled Dynamical Systems[1]

Dynamical equations arising in a number of physical areas typically involve many dependent variables as well as numerous parameters. In some cases these equations may contain a dominant dependent variable (e.g., the temperature in flame systems, etc.), and the consequences of such an identification are examined in this paper. Particular emphasis is placed on the behavior of dynamical Green's functions and system sensitivity coefficients with respect to the parameters residing in the particular model. In the case of a single dominant dependent variable for a system of ordinary differential equations, it is possible to reduce the Green's function matrix to knowledge of one of its columns and often to one independent element. Furthermore, when there are N dependent variables and M parameters, the $N \times M$ matrix of sensitivity coefficients reduces to knowledge of only two characteristic vectors of lengths N and M, respectively, These various reductions are referred to as scaling relations and self-similarity conditions. The consequences of a dominant dependent variable are illustrated with examples drawn from various areas of combustion and kinetics modelling. A brief discussion in the Appendix is also presented on similar organizing principles in multidominant dependent variable systems and cases described by partial differential equations.

2.   A General Analysis of Exact Lumping in Chemical Kinetics[2]

A general analysis of exact lumping is presented. This analysis can be applied to any reaction system with n species described by a set of first order differential equations $dy/dt = f(y)$, where y is an n-dimensional vector; $f(y)$ is an arbitrary n-dimensional function vector. Here we consider lumping by means of an $\hat{n} \times n$ real constant matrix M with rank $\hat{n}(\hat{n} < n)$. It is found that a reaction system is exactly lumpable if and only if there exist nontrivial fixed invariant subspaces M of the transpose of the Jacobian matrix $J_T(y)$ of $f(y)$, no matter what value y takes and the corresponding eigenvalues are the same for $J_T(y)$ and $J_T(M \bar{M}y)$. Here the rows of M are the basis vectors of M and $\bar{M}$ is any generalized inverse of M satisfying $M \bar{M} = I_n$ with I_n being the n-identity matrix. The fixed invariant subspaces of $J^T(y)$ can be obtained either from the simultaneously invariant subspaces of all A_k, where the A_k's form the basis of decomposition of $J^T(y)$, or by determining the fixed $Ker(\pi_i(J^T(y) - \lambda_i I_n)^{r_i} \pi_j[(\sigma_j + r_j) I_n - 2\sigma_j J^T(y)$ $+ (J^T(y))^2]^{r_j})$, where λ_i, $\sigma_j \pm ir_j$ are the real and nonreal eigenvalues of $J^T(y)$ and λ_i, σ_j and r_j are usually functions of y_i and r_j are non-negative integers. The kinetic equations of the lumped system can be described as $d\hat{y}/dt = Mf(M\hat{y})$. This method is illustrated by some simple examples.

3.   Identifiability and Distinguishability of First-order Reaction Systems[3]

By following the kinetics of a reaction through the use of certain classes of measurable quantities instead of the concentration of all species, neither the parameter values nor the reaction scheme is necessarily unique. Identifiability deals with the problem of determining whether an experiment is able to supply the desired information on the parameters of an assumed kinetic model, whereas indistinguishability means that two different reaction schemes generate the same values for the observed quantities in any possible experiment. This paper examines

these issues for the case of first-order reaction systems, and both problems are solved by the same analytical tools. The method involving Laplace transforms is conceptually simple, is easy to apply, and is also used to derive simple rules to test distinguishability of reaction schemes. Another approach based on similarity transformations is used to generate all the first-order reaction schemes that are indistinguishable from a given one.

4. **Parameter Space Mapping of First-Order Linear Ordinary Differential Equations[4]**

A Lie group formalism for global parameter space mapping of ordinary differential equations, described in a preceding paper, is developed here. The need for such mapping arises in a variety of physical contexts. The procedure is demonstrated on, but not restricted to, the system of coupled equations $\dot{x} - cx$. The Lie group generators are obtained exactly from both the time-independent and time-dependent generating equations. The transformations obtained from these generators leave the system of differential equations invariant. The time-indpendent transformations map any solution of the linear system $\dot{x} - xc$ into any other solution with the same frequency or time constant. The time-dependent transformations interconvert solutions with different frequencies and/or small time constants. Any solution of $\dot{x} - xc$ can be mapped into any solution of $\dot{x} - c'x$. Thus the behavior of $x(t)$ can be examined as a function of changes in any of the system parameters, or in the initial conditions, $x(0)$. As an example, one of the time-dependent mappings demonstrates the continuous transformation of oscillator solutions into nonoscillatory ones, and vice versa.

5.   Global Sensitivity Analysis of Nonlinear Chemical Kinetics Equations
     Using Lie Groups: I.   Determination of One-parameter Groups[5]

We introduce one-parameter groups of transformations that affect wide-ranging

changes in the rate constants and input/output fluxes of homogeneous chemical

reactions involving an arbitrary number of species in reactions of zero, first and

second order.

Each one-parameter group is required to convert every solution of such

elementary rate equations into corresponding solutions of a one-parameter family of

altered elementary rate equations.

The generators of all allowed one-parameter groups are obtained for systems

with N species using an algorithm which exactly determines their action on the rate

constants, and either exactly determines or systematically approximates their

action on the concentration. Compounding the one-parameter groups yields all

many-parameter groups of smooth time-independent transformations that interconvert

elementary rate equations and their solutions.

6.   Complications of One-Step Kinetics for Moist CO Oxidation[6]

The one-step reaction mechanism, $CO + \frac{1}{2} O_2 \rightarrow CO_2$ with

$$d[CO]/dt = -k_{ov}[CO]^a[H_2O]^b[O_2]^c$$

which is frequently used in combustion problems when simplified chemistry is

necessary, is numerically studied in order to (i) define its limitations (and

therefore usage) and (ii) understand the chemical and physical reasons for these

limitations. The analysis is carried out with the aid of a validated

comprehensive, elementary reaction mechanism for moist CO oxidation and by

specialized sensitivity coefficients which correlate the parameters of the global

model to the parameters of the elementary model. The results confirm many of the

previous, empirically derived, literature models and show the overall rate

constant, as a function of temperature, to exhibit non-Arrhenius kinetics and to be dependent on pressure and mixture equivalence ratio. More importantly, models derived from temporally reacting systems are shown to be improper for use in modelling systems reacting with transport phenomena. The specialized sensitivity coefficients are used to explain these complex behaviors in the overall model. For the temporal system, these coefficients show that the global model must be able to account for dissociation and equilibration at high temperatures, for explosion phenomena in the intermediate temperatures, and for reaction of carbon monoxide with both the hydroxyl radical and hydroperoxy radical at low temperatures. Lastly, methods for modifying the existing model or for developing a new model are suggested.

7.   Elementary Model Reduction of Carbon Monoxide Kinetics

In our previous studies, normalized elementary sensitivity coefficients have been used to determine the relative importance of elementary reactions or certain groups of reactions in comprehensive mechanisms. In this study, we have extended this methodology by using the principal component analysis method in order to systematically reduce the size of the original comprehensive mechanism. Briefly, this methodology is based on a least squares fit approach by first defining the response function, Q, as:

$$Q(\underline{\alpha}) = \sum_{j=1}^{a} \sum_{i=1}^{m} \left[\frac{C_i(t_j,\underline{\alpha}) - C_i(t_j,\underline{\alpha}^\circ)}{C_i(t_j,\underline{\alpha}^\circ)} \right]^2$$

where α° is the nominal values of the parameters, then by introducing the classical Gauss-approximation to yield $Q(\underline{\dot{\alpha}}) = \tilde{Q}(\underline{\dot{\alpha}}) = (\Delta\dot{a})^T \underline{S}^T \underline{S}(\Delta\dot{\alpha})$ where $\dot{a}_j = \ln \alpha_j$, and finally by performing an eigenvalue-eigenvector decomposition on the resulting cross-product matrix $\underline{S}^T\underline{S}$. Eigenvectors corresponding to small eigenvalues

indicate unimportant reactions, thereby enabling one to optimally reduce the mechanism.

Along these lines, we have continued our previous work by applying this methodology to the $CO/H_2/O_2$ reaction mechanism. A large number of isothermal temporal problems were numerically run to generate a data base which would be representative of combustion environment:. The data base covered a temperature range from 800 to 1800 K, several equivalence ratios from lean to rich conditions, and several pressures. The principal component analysis was applied to this data base to determine the minimum reaction set that would reproduce all the original species concentrations within 2%.

The results showed that the original 52 reaction mechanisms could be successfully reduced to one consisting of 27 reactions while retaining all 12 species in the model.

Obviously, this reduction is still not practical for use in large multidimensional codes. The necessary further reductions are proceeding along several directions. First, the constraint of retaining all species will be lifted. Our earlier research has shown that in addition to the major reactants and products, two intermediate species are necessary in the model. Secondly, we have also found that in more complex environments, such as adiabatic premixed flames, the underlying chemical processes are much more coupled (namely through the heat release of the reaction) and hence, such problems are anticipated to be more directly lumpable.

List of Publications Citing AFOSR Under This Research

1. H. Rabitz and M.D. Smooke, J. Phys. Chem., 91, 1110 (1988).

2. G. Li and H. Rabitz, Chem. Eng. Sci., in press.

3. S. Vajda and H. Rabitz, J. Phys. Chem., 92, 701, (1988).

4. L.M. Hubbard, C. Wulfman and H. Rabitz, J. Phys. Chem., 90, 2273 (1986).

5. H. Rabitz and C. Wulfman, J. Math. Chem., in press.

6. R.A. Yetter, F.L. Dryer and H. Rabitz, presented at the Twenty-First Symposium (International) on Combustion, Munich, West Germany, August 3-8, 1986.

Personnel

Mr. Genyuan Li, graduate student
Dr. Sandor Vajda, postdoctoral associate
Dr. Carl Wulfman, consultant

Presentations Associated with the Research

R. Yetter - Workshop on Developing a Predictive Capability for
CO Formation in Fires, National Institute of Standards
and Technology, Clearwater, Florida, December 1988.

H. Rabitz* - New York University
Aerodyne Research Inc.
Sandia Laboratories
City College of New York
Dartmouth College
Computer Simulations Conference
Picatinny Arsenal
Cummins Engine Company
University of Texas, Austin
Stanford University
Aerospace Corporation
* Dr. Rabitz' various presentations were on kinetic
lumping, reduction, and sensitivity analysis.

Inventions - none